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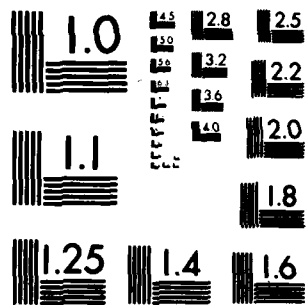   DEC 81   F L CARTER
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20. ABSTRACT *(Continue on reverse side if necessary and identify by block number)*

An exact analytic solution has been derived for the transmission of electrons through a series of up to six square potential steps. From these an algorithm is derived which readily gives the solution for any arbitrary number of square potential steps.

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CONTENTS

ELECTRON TRANSMISSION THROUGH AND REFLECTION BY AN

ARBITRARY SET OF SQUARE POTENTIAL STEPS

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INTRODUCTION

Traditionally solutions of the Schrodinger wave equation for square-well and step-function potentials have served primarily heuristic and pedagogical purposes. More recently, however, advances in the use of multibeam evaporators have made possible the growth of layered semiconductors with layers only a few Angstroms thick. In addition we have proposed[1] that analogues to NAND and NOR switches might be possible at the molecular size level. That proposal relies on the quasi-classical work of Pschenichnov[2] who for a one dimensional system of identical potential barriers anticipated the existence of an electron tunnel effect.

The tunnel effect occurs when the electron's energy, ω, matches that of a pseudo-stationary state, E_n, (i.e., a virtual level) related to an energy level of the well between barriers, when ω is less than the height of the barriers. The work of Pschenichnov[2] suggests that where this condition is met (i.e., $\omega = E_n$) then the transmission coefficient T is equal to 1; in other words, at this energy, the barriers are perfectly transparent. However, at a small energy mismatch, transmission falls exponentially with the number of barriers. The extremely rapid decline in electron transmission with the energy mismatch provides the basis for a switching mechanism assuming that one is perturbing one or more of the potential wells or barriers and hence disturbing the energy level of the pseudo-stationary state. Both the layered semiconductors and the molecular tunnelling as conceived[1] can be reasonably treated as a one dimensional problem (the approach taken here). In addition, the results obtained below may be useful for understanding electron transport and scattering along a polymer chain with a non-periodic distribution of substituents or conjugation.

Derivation

From the author's[3] earlier result involving a periodic set of an arbitrary number of potential step functions per unit cell it seemed reasonable that an exact expression might be achievable for electron transmission past an arbitrary number of square wells and barriers. That possibility is vindicated in this paper; both the derivation and the generalized analytic expression are given for the transmission coefficient T of an electron past any number of step-function potential changes. The method is classical textbook (see Schiff [4]).
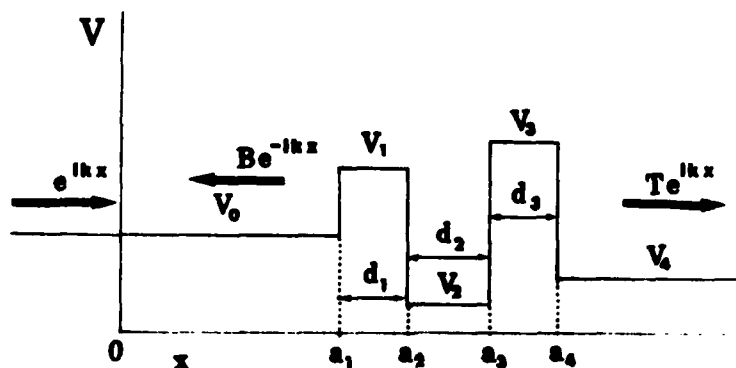

Fig. 1. Square well (and barrier) potentials of width d_i and depth (height) V_i in the path of a unit wave approaching from the extreme left.

Before developing the expression for perfect transmission, it is very useful to understand the relationships for the wave function in the regions of adjacent potentials. The time independent Schrodinger wave equation in atomic units is

$$\frac{d^2\psi}{dx^2} + 2[E - V(x)]\psi = 0 \qquad \text{Eq. 1}$$

where for constant potential V the wave function $\Psi(x)$ can be readily written as

$$\Psi_n(x) = A_n e^{i\beta_n x} + B_n e^{-i\beta_n x} \qquad \text{Eq. 2}$$

correspondingly to waves of energy $E = \omega$ moving to the right and left with amplitudes A_n and B_n respectively. The exponential multiplier β_n is determined by substituting Ψ_n (Eq. 2) in the differential wave equation (Eq. 1); while the coefficients A_n, B_n are determined by joining Ψ_n and its first derivative $d\Psi_i/dx$

continuously at each step position a_n of Fig. 1. With $\Psi_n(x)$ corresponding to the wave function with $a_n \leq x < a_{n+1}$ the continuity requirements give two equations for each potential step at the positions a_n; thus,

functional continuity

$$A_{n-1}e^{i\beta_{n-1}a_n} + B_{n-1}e^{-i\beta_{n-1}a_n} = A_n e^{i\beta_n a_n} + B_n e^{-i\beta_n a_n} \qquad \text{Eq. 3}$$

slope continuity

$$\beta_{n-1}A_{n-1}e^{i\beta_{n-1}a_n} - \beta_{n-1}B_{n-1}e^{-i\beta_{n-1}a_n} = \beta_n A_n e^{i\beta_n a_n} -$$

$$\beta_n B_n e^{-i\beta_n a_n} \qquad \text{Eq. 4}$$

Obviously, A_n and B_n can be expressed as a matrix multiplication M_n of the coefficients A_{n-1} and B_{n-1}

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M_n \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \qquad \text{Eq. 5}$$

This equation can be easily generalized, as was done by Pschenichnov[2] for his quasi-classical approach, to the form:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M_n \cdot M_{n-1} \cdots M_2 \cdot M_1 \begin{pmatrix} A_o \\ B_o \end{pmatrix} \qquad \text{Eq. 6}$$

where n is the counting index of the potential steps. Clearly since a well of finite barrier requires at least two potential steps, the matrices must be grouped at least by pairs to be compared with Pschenichnov's results.

New Results

The matrices M_n and their successive products, however, are complex (in both senses) and are awkward to write down. It is more convenient to discuss their products like

$$\prod_{1}^{n} M_i \quad \text{and} \quad \prod_{k+1}^{n} M_i$$

in terms of the new and much simpler analytic expressions $U_{no}^{\pm}$ and $V_{no}^{\pm}$ to be given explicitly below for the first time for various n up to 6.

In these terms $\prod_{1}^{n} M_i$ and $\prod_{k+1}^{n} M_i$ may be related to Eqs. 7 and 8 and Eqs. 9 and 10, respectively. The relationship between the coefficients A_n, B_n and A_O, B_O in terms of $U_{nk}^{\pm}$ and $V_{ko}^{\pm}$ etc. is indicated by Eqs. 11 and 12.

The $U_{no}^{\pm}$ and $V_{no}^{\pm}$ are to be given in Table 1 in terms various β_i, S_i, and C_i as defined below where on the left the electron energy ω is greater than the potential V_i, etc:

Low Potential	High Potential
$V_i \leq \omega$	$V_i > \omega$
$\beta_i = \sqrt{\omega - V_i}$	$\beta_i = \sqrt{V_i - \omega}$
$C_i = \cos \beta_i d_i$	$C_i = \cosh \beta_i d_i$
$S_i = \sin \beta_i d_i$	$S_i = \sinh \beta_i d_i$

Although $U_{no}^{\pm}$ and $V_{no}^{\pm}$ functions rapidly become rather complex for increasing n in fact they are rather simple once understood, and they can readily be generalized. The verbal algorithm for doing so will be indicated after the formula for the transmission coefficient T is developed.

In terms of Fig. 1 and the coefficient pairs A_O, B_O and A_n, B_n the calculation for T is readily described. Approaching the first potential step at A_1 from infinity is the unit wave $e^{i\beta x}$, thus $A_O = 1$. Reflected from that first potential step is the wave with unknown amplitude $B = B_O$. The coefficient of the wave that gets through to the region V_4, $x > a_4$ is the desired transmission amplitude T. Note that there is no wave coming from the right in this region; hence $A_n = T$ and $B_n = 0$. From Eqs. 7 and 8 and the coefficients just specified one can then readily obtain Eq. 13

$$T = A_n = A_O \frac{e^{i(\beta_o a_1 - \beta_n a_n)}}{2} \frac{\left[(U_{no}^{+})^2 + (V_{no}^{+})^2 - (U_{no}^{-})^2 - (V_{no}^{-})^2\right]}{U_{no}^{+} - i V_{no}^{+}} \qquad \text{Eq. 13}$$

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GENERATE GENERAL RULE FOR COEFFICIENTS

$$A_n \cdot 2 \cdot e^{i\beta_n a_n} = [U_{no}^+ + iV_{no}^+] \, A_o e^{i\beta_o a_1} + [U_{no}^- - iV_{no}^-] \, B_o e^{-i\beta_o a_1} \qquad \text{Eq. 7}$$

$$B_n \cdot 2 \cdot e^{-i\beta_n a_n} = [U_{no}^- + iV_{no}^-] \, A_o e^{i\beta_o a_1} + [U_{no}^+ - iV_{no}^+] \, B_o e^{-i\beta_o a_1} \qquad \text{Eq. 8}$$

$$A_n \cdot 2 \cdot e^{i\beta_n a_n} = [U_{nk}^+ + iV_{nk}^+] \, A_k e^{i\beta_k a_{k+1}} + [U_{nk}^- - iV_{nk}^-] \, B_k e^{-i\beta_k a_{k+1}} \qquad \text{Eq. 9}$$

$$B_n \cdot 2 \cdot e^{-i\beta_n a_n} = [U_{nk}^- + iV_{nk}^-] \, A_k e^{i\beta_k a_{k+1}} + [U_{nk}^+ - iV_{nk}^+] \, B_k e^{-i\beta_k a_{k+1}} \qquad \text{Eq. 10}$$

Substitute for $A_k + B_k$

$$A_n \cdot 2 \cdot e^{i\beta_n a_n} = A_o e^{i\beta_o a_1} \left[\frac{e^{i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^+ + iV_{nk}^+)(U_{ko}^+ + iV_{ko}^+) + \frac{e^{-i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^- - iV_{nk}^-)(U_{ko}^- + iV_{ko}^-) \right] +$$

$$+ B_o e^{-i\beta_o a_1} \left[\frac{e^{i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^+ + iV_{nk}^+)(U_{ko}^- - iV_{ko}^-) + \frac{e^{-\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^- - iV_{nk}^-)(U_{ko}^+ - iV_{ko}^+) \right] \qquad \text{Eq. 11}$$

$$B_n \cdot 2 \cdot e^{-i\beta_n a_n} = A_o e^{i\beta_o a_1} \left[\frac{e^{i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^- + iV_{nk}^-)(U_{ko}^+ + iV_{ko}^+) + \frac{e^{-i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^+ - iV_{nk}^+)(U_{ko}^- + iV_{ko}^-) \right] +$$

$$+ B_o e^{-i\beta_o a_1} \left[\frac{e^{i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^- + iV_{nk}^-)(U_{ko}^- - iV_{ko}^-) + \frac{e^{-i\beta_k(a_{k+1}-a_k)}}{2} (U_{nk}^+ - iV_{nk}^+)(U_{ko}^+ - iV_{ko}^+) \right] \qquad \text{Eq. 12}$$

TABLE I OF COEFFICIENTS $U_{no}^{\pm}$ AND $V_{no}^{\pm}$

$n = 1$

$U_{no}^{\pm} = (1 \pm \frac{B_o}{B_1})$

$V_{10}^{+} = V_{10}^{-} = 0$

$n = 2$

$U_{20}^{\pm} = (1 \pm \frac{B_o}{B_2})c_1$

$V_{20}^{\pm} = -(\frac{B_o}{B_1} \pm \frac{B_1}{B_2})s_1$

$n = 3$

$U_{30}^{\pm} = (1 \pm \frac{B_o}{B_3})c_1c_2 - (\frac{B_1}{B_2} \pm \frac{B_o}{B_1}\frac{B_2}{B_3})s_1s_2$

$V_{30}^{+} = -(\frac{B_o}{B_2} \pm \frac{B_2}{B_3})c_1s_2 + (\frac{B_o}{B_1} \pm \frac{B_1}{B_3})s_1c_2$

$n = 4$

$U_{40}^{\pm} = (1 \pm \frac{B_o}{B_4})c_1c_2c_3 - (\frac{B_2}{B_3} \pm \frac{B_oB_3}{B_2B_4})c_1s_2s_3 - (\frac{B_1}{B_3} \pm \frac{B_oB_3}{B_1B_4})s_1c_2s_3 - (\frac{B_1}{B_2} \pm \frac{B_oB_2}{B_1B_4})s_1s_2c_3$

$V_{40}^{\pm} = -(\frac{B_o}{B_3} \pm \frac{B_3}{B_4})c_1c_2s_3 + (\frac{B_o}{B_2} \pm \frac{B_2}{B_4})c_1s_2c_3 + (\frac{B_o}{B_1} \pm \frac{B_1}{B_4})s_1c_2c_3 - (\frac{B_o}{B_1}\frac{B_2}{B_3} \pm \frac{B_1B_3}{B_2B_4})s_1s_2s_3$

$n = 5$

$U_{50}^{\pm} = (1 \pm \frac{B_o}{B_5})c_1c_2c_3c_4 - (\frac{B_3}{B_4} \pm \frac{B_oB_4}{B_3B_5})c_1c_2s_3s_4 - (\frac{B_2}{B_4} \pm \frac{B_oB_4}{B_2B_5})c_1s_2c_3s_4 - (\frac{B_2}{B_3} \pm \frac{B_oB_3}{B_2B_5})c_1s_2s_3c_4 - (\frac{B_1}{B_4} \pm \frac{B_oB_4}{B_1B_5})s_1c_2c_3s_4 - (\frac{B_1}{B_3} \pm \frac{B_oB_3}{B_1B_5})s_1c_2s_3c_4 - (\frac{B_1}{B_2} \pm \frac{B_oB_2}{B_1B_5})s_1s_2c_3c_4$

$V_{50}^{\pm} = -(\frac{B_o}{B_4} \pm \frac{B_4}{B_5})c_1c_2c_3s_4 + (\frac{B_o}{B_3} \pm \frac{B_3}{B_5})c_1c_2s_3c_4 + (\frac{B_o}{B_2} \pm \frac{B_2}{B_5})c_1s_2c_3c_4 + (\frac{B_o}{B_1} \pm \frac{B_1}{B_5})s_1c_2c_3c_4 - (\frac{B_o}{B_2}\frac{B_3}{B_4} \pm \frac{B_2B_4}{B_3B_5})c_1s_2s_3s_4 - (\frac{B_o}{B_1}\frac{B_3}{B_4} \pm \frac{B_1B_4}{B_3B_5})s_1c_2s_3s_4 - (\frac{B_o}{B_1}\frac{B_2}{B_3} \pm \frac{B_1B_3}{B_2B_5})s_1s_2c_3s_4 - (\frac{B_oB_2}{B_1B_4} \pm \frac{B_1B_4}{B_2B_5})s_1s_2s_3c_4$

TABLE I OF COEFFICIENTS $U^{\pm}_{no}$ AND $V^{\pm}_{no}$ (CONT'D)

n = 6

$$U^{\pm}_{60} = (1 \pm \frac{B_0}{B_6})C_1C_2C_3C_4C_5 - (\frac{B_4}{B_5} \pm \frac{B_0B_5}{B_4B_6})C_1C_2C_3C_4S_5 - (\frac{B_3}{B_5} \pm \frac{B_0B_5}{B_3B_6})C_1C_2C_3S_4C_5 - (\frac{B_2}{B_5} \pm \frac{B_0B_5}{B_1B_6})C_1S_2C_3C_4C_5$$

$$- (\frac{B_1}{B_5} \pm \frac{B_0B_5}{B_1B_6})S_1C_2C_3C_4C_5 - (\frac{B_3}{B_4} \pm \frac{B_0B_4}{B_3B_6})C_1C_2S_3S_4C_5 - (\frac{B_2}{B_4} \pm \frac{B_0B_4}{B_2B_6})C_1S_2C_3S_4C_5 - (\frac{B_1}{B_4} \pm \frac{B_0B_4}{B_1B_6})S_1C_2C_3S_4C_5$$

$$- (\frac{B_2}{B_3} \pm \frac{B_0B_3}{B_2B_6})C_1S_2S_3C_4C_5 - (\frac{B_1}{B_3} \pm \frac{B_0B_3}{B_1B_6})S_1C_2S_3C_4C_5 - (\frac{B_1}{B_2} \pm \frac{B_0B_2}{B_1B_6})S_1S_2C_3C_4C_5 + (\frac{B_2B_4}{B_3B_5} \pm \frac{B_0B_3B_5}{B_2B_4B_6})C_1S_2S_3S_4S_5$$

$$+ (\frac{B_1B_4}{B_3B_5} \pm \frac{B_0B_3B_5}{B_1B_4B_6})S_1C_2S_3S_4S_5 + (\frac{B_1B_3}{B_2B_5} \pm \frac{B_0B_2B_5}{B_1B_3B_6})S_1S_2C_3S_4S_5$$

$$+ (\frac{B_1B_3}{B_2B_4} \pm \frac{B_0B_2B_4}{B_1B_3B_6})S_1S_2S_3S_4C_5$$

$$V^{\pm}_{60} = (\frac{B_0}{B_5} \pm \frac{B_5}{B_6})C_1C_2C_3C_4S_5 + (\frac{B_0}{B_4} \pm \frac{B_4}{B_6})C_1C_2C_3S_4C_5 + (\frac{B_0}{B_3} \pm \frac{B_3}{B_6})C_1C_2S_3C_4C_5 + (\frac{B_0}{B_2} \pm \frac{B_2}{B_6})C_1S_2C_3C_4C_5 +$$

$$+ (\frac{B_0}{B_1} \pm \frac{B_1}{B_6})S_1C_2C_3C_4C_5 - (\frac{B_0B_4}{B_3B_5} \pm \frac{B_2B_5}{B_4B_6})C_1C_2S_3S_4S_5 - (\frac{B_0B_3}{B_2B_5} \pm \frac{B_3B_5}{B_3B_6})C_1S_2S_3C_4S_5 - (\frac{B_0B_3}{B_1B_5} \pm \frac{B_1B_5}{B_3B_6})S_1C_2S_3C_4S_5 +$$

$$- (\frac{B_0B_4}{B_3B_5} \pm \frac{B_2B_4}{B_4B_6})C_1S_2S_3S_4C_5 - (\frac{B_0B_3}{B_1B_5} \pm \frac{B_1B_5}{B_3B_6})S_1C_2S_3C_4S_5 - (\frac{B_1B_4}{B_3B_6} \pm \frac{B_1B_4}{B_3B_6})S_1C_2S_3S_4$$

$$- (\frac{B_0B_4}{B_2B_4} \pm \frac{B_2B_4}{B_3B_6})C_1S_2S_3S_4C_5 - (\frac{B_0B_3}{B_1B_5} \pm \frac{B_1B_5}{B_3B_6})S_1C_2S_3C_4S_5 - (\frac{B_0B_2}{B_1B_4} \pm \frac{B_1B_4}{B_3B_6})S_1C_2S_3S_4$$

$$- (\frac{B_0B_2}{B_1B_3} \pm \frac{B_1B_3}{B_2B_6})S_1S_2C_3C_4S_5 - (\frac{B_0B_2}{B_1B_6} \pm \frac{B_1B_5}{B_2B_6})S_1S_2S_3C_4C_5$$

$$+ (\frac{B_0B_2B_4}{B_1B_3B_5} \pm \frac{B_1B_3B_5}{B_2B_4B_6})S_1S_2S_3S_4S_5$$

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then with $A_0 = 1$ we have for the transmission coefficient

$$|T|^2 = \frac{\left[(U_{no}^+)^2 + (V_{no}^+)^2 - (U_{no}^-)^2 - (V_{no}^-)^2 \right]^2}{4[(U_{no}^+)^2 + (V_{no}^+)^2]} \qquad \text{Eq. 14}$$

Equation 14 informs us that the transmission is maximized when U_{no}^+ and V_{no}^+ approach zero while the numerator remains finite. Table 2 indicates the behavior of the numerator for the first few values of n, the number of step potential changes. Generally it is not a fast varying function.

The relationship of the function U_{no}^+ (obtained here) to the solution of the wave equation for a periodic set of square well potentials is rather interesting. This is readily illustrated for the Konig-Penny square well model[3] when expressed in the notation above. Given that k is the wave vector and c is the unit cell length we have [3]:

$$\cos kc = C_1 C_2 - \frac{1}{2} \left[\frac{B_1}{B_2} + \frac{B_2}{B_1} \right] S_1 S_2 \qquad \text{Eq. 15}$$

This may be compared readily with U_{no}^+:

$$U_{30}^+ = (1 + \frac{B_0}{B_3}) C_1 C_2 - \left[\frac{B_1}{B_2} + \frac{B_0}{B_1} \frac{B_2}{B_3} \right] S_1 S_2 \qquad \text{Eq. 16}$$

Periodicity after two potential steps requires that $\beta_0 = \beta_3$ so that one may clearly combine eqs. 15 and 16 to form

$$\cos kc = U_{30}^+ / 2 \qquad \text{Eq. 17}$$

Given n-1 steps per unit cell, Eq. 17 may be generalized to

$$\cos kc = U_{no}^+ / 2 \qquad \text{Eq. 18}$$

Remembering elementary band theory we note that allowed bands exist only when $\cos kc \leq 1$ and forbidden gaps occur otherwise. Now when $U_{no}^+ = 0$ then a virtual state exists, which may be related via Eq. 18 to the case of $\cos kc = 0$, i.e., the center of the allowed bands.

TABLE 2

TRANSMISSION COEFFICIENT NUMERATOR

$$N_{no} = (U^+_{no})^2 + (V^+_{no})^2 - (U^-_{no})^2 - (V^-_{no})^2$$

$$N_{10} = 4 \frac{\beta_0}{\beta_1}$$

$$N_{20} = 4 \frac{\beta_0}{\beta_2} (C_1{}^2 + S_1{}^2)$$

$$N_{30} = 4 \frac{\beta_0}{\beta_3} \left[C_1{}^2 C_2{}^2 + S_1{}^2 S_2{}^2 + S_2{}^2 C_1{}^2 + S_1{}^2 S_2{}^2 \right]$$

This then agrees well with one's expectations and to that extent supports the conclusions of Pschenichnov for the tunnelling of electrons through periodic barriers.

Algorithm for $U^\pm_{no}$ and $V^\pm_{no}$

Table 1 shows that in $U^\pm_{no}$ only even numbers, m, of S_i occur; further that the number of such terms is $\binom{n-1}{m} = \frac{(n-1)!}{(n-1-m)m!}$, that is, all possible combinations of n-1 positions take m at a time. The sign in front of a term like $(\frac{\beta_4}{\beta_5} \pm \frac{\beta_0}{\beta_4} \frac{\beta_5}{\beta_6}) C_1 C_2 C_3 S_4 S_5$ is + if mod (m DIV 2,2) is zero and negative otherwise (where DIV means integer divide). In the β_i ratios, only β_i corresponding to the S_i occur. In the lead β ratio, the first β_i occurs in the numerator, the second in the denominator, and the alteration continues. The second β_i ratio is the reciprocal of the first ratio multiplied by β_0/β_n.

Two differences occur in the case of the $V^\pm_{no}$ function. First, m is only odd. The second occurs in the β_i ratios. In the first ratio one always starts with β_0, whereas in the second ratio the first possible one is β_1 and the last β_i factor is always β_n.

Summary

Using a time independent method the analytic formula for the transmission of an electron through an arbitrary number of step potential changes has been derived. An algorithm has been given for writing down the formula for any number of potential steps. In addition the virtual levels have been identified with the allowed band centers in a corresponding case of n-1 potential step changes per unit cell of a periodic array.

The existence of a generalized analytic solution, now available for the first time is important not only in terms of investigating the details of electron tunnelling in one and two dimensional molecular switches but also in terms of electron conduction in polymers. Thus, while eq. 18 is applicable to crystalline or periodic polymers, Eq. 14 will be useful for understanding and modeling non-crystalline or non-periodic materials as might occur in multiple co-polymers in the presence or absence of a small electric field.

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